

chain nodes:

13 14 15 16 17 18 19 20 21 22 27 28 29

ring nodes:

1 2 3 4 5 6 7 8 9 10 11 12

chain bonds:

2-16 5-13 9-15 12-27 13-14 13-15 16-17 17-18 18-19 19-20 19-21 21-22 27-28 28-29

ring bonds:

1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12

exact/norm bonds:

2-16 7-8 7-12 8-9 9-10 9-15 10-11 11-12 12-27 13-14 13-15 18-19 19-20 27-28

exact bonds:

5-13 16-17 17-18 19-21 21-22 28-29

normalized bonds:

1-2 1-6 2-3 3-4 4-5 5-6

## Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom 12:Atom 13:CLAS\$14:CLAS\$15:CLAS\$16:CLAS\$17:CLAS\$18:CLAS\$19:CLAS\$20:CLAS\$21:CLAS\$22:CLAS\$27:CLAS\$28:CLAS\$29:CLAS\$20:CLAS